Int J Clin Exp Med 2018;11(8):8267-8274
www.ijcem.com /ISSN:1940-5901/IJCEM0077156

Original Article

Comparison of metabolites profiling between *Lycium chinense* and *Taxus chinensis* by GC/TOF MS

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Received September 17, 2017; Accepted May 31, 2018; Epub August 15, 2018; Published August 30, 2018

Abstract: *Lycium chinense* (Goji) and *Taxus chinensis* (Hongdoushan) are two important traditional Chinese medicines (TCMs), which are usually used for maintaining the health due to their significant pharmaceutical interests including anticancer properties and antioxidant activities. However, there are very few metabolomics studies on biological activities or bio-active components for these two TCMs. In the present study, we for the first time performed metabolic profiling of two important TCMs by a non-targeted metabolomic technology, GC/TOF MS. Totally 321 metabolites were identified in *Lycium chinense*, while a total of 339 metabolites were found in *Taxus chinensis*. The results here revealed a comprehensive metabolome for both TCMs. Further analysis including K-Medians clustering analysis and principal component analysis (PCA) revealed a remarkable metabolic variation between these two TCMs. More importantly, six significantly changed metabolites ($p \leq 0.05$) were determined between *Lycium chinense* and *Taxus chinensis*, which may play important roles on their specific significant pharmaceutical interests including anticancer property. Altogether, the results here for the first time presented significant bioactive components in *Lycium chinense* and *Taxus chinensis*. And meanwhile, it may provide new insights into their potentials in the prevention and treatment of various diseases including cancer.

Keywords: Anticancer, bioactive components, *Lycium chinense*, *Taxus chinensis*, traditional Chinese medicine (TCM)

Introduction

Traditional Chinese medicines (TCMs), or so called Chinese herbal medicines (CHMs), have a long history dating back more than four thousand years ago in China. They are traditionally used for maintaining the health of peoples by reducing the risk of chronic diseases and acting as powerful antioxidants [1]. Currently, TCMs are getting more and more popular in the whole world due to their reliable therapeutic efficacy. Particularly, China's pharmacologist Tu Youyou responsible for the discovery of artemisin, was awarded the Nobel Prize in 2015, which highlighted more attentions to TCM researches and its potentials [2].

"-Omics" technologies including genomics, transcriptomics, proteomics, and metabolomics, which have opened a new gate in the study of TCMs, enabling the illustration of TCMs from a more systematic view [3]. For example, Zheng *et al*. (2011) reported the genome sequence of the type species Cordyceps militaris, which may facilitate the exploitation of medicinal compounds produced by the fungus [4]. Moreover, by the 454 pyrosequencing technology, a total of 195, 088 high-quality reads have been determined in *Bupleurum chinense* DC. And more importantly, two P450s and three UGTs have been identified as the most likely candidates involved in saikosaponin biosynthesis [5]. Meanwhile, Lum *et al.* (2002) employed a proteomic approach to establish two-dimensional electrophoresis (2-DE) maps from the American ginseng main root, different parts of Oriental ginseng and Oriental ginseng culture cells [6]. The results identified common and specific protein spots, which may help to speed up the identification process.

Additionally, another emerging and potentially powerful tool, metabolomics, has been widely used to reveal the theory behind the evidence-based Chinese medicine including Chinese medicine syndromes, action of Chinese medicine, preventive treatment, Chinese medical formulae and acupuncture efficacy [7-12]. The technology also has the potential for disease diagnosis, screening of new drugs, quality control, evaluation of the efficacy and safety, as well as the discovery of novel biomarkers of chemical therapeutics or TCM products [8, 9]. For instance, by using AFLP based genetic fingerprinting and GC-TOF/MS-based metabolic fingerprinting, Duan *et al.* (2012) characterized Chinese medicinal material Huangqi, which showed growth locations have greater impacts on the metabolite composition and quantity than the genotypes in Menggu Huangqi [10]. Meanwhile, three AFLP markers and eight metabolic markers have finally been determined to be DNA markers and biomarkers to distinguish the two herb materials (Mojia Huangqi and Menggu Huangqi).

TCMs contains hundreds of or even thousands of compounds, which have been proved to have the activities in clinical trials or modern pharmacological studies [13]. While the identity of the bioactive compounds in TCMs remains a research hotspot. So far, many applications using metabolomics strategy have been reported for screening bioactive components in TCMs including Ginseng, Huangqi, and Sanchi [7, 10]. In the present study, taking advantage of a non-targeted metabolomic analysis by GC/TOF MS, we for the first time performed metabolic profiling of *Lycium chinense* (Goji) and *Taxus chinensis* (Hongdoushan). These two important TCMs: are usually mixed for soaked wine in China, which are supposed to maintain beauty and keep young, as well as health care conditioning. The results here revealed a comprehensive metabolome (including bioactive compounds) for both TCMs, and meanwhile, a remarkable metabolic variation was observed between the two groups. Altogether, the study here not only presented a non-targeted metabolite profiling as a useful approach for discriminating these two TCMs (*Lycium chinense* and *Taxus chinensis*), but also provided new insights into their potentials in reducing the risk of diseases including cancer.

Materials and methods

Materials collection

The commonly available seeds of *Lycium chinense* were bought from the primary regional producers in Ningxia (located in Loss Plateau, China), which is the most popular and best-selling in the foods market. The plants of *Taxus chinensis,* so called *Taxus wallichiana* var. mairei (Lemée & Levéillé) L. K. Fu & Nan Li, were grown in a local farm at Jiangxi Province, South China. Three repeats of *Lycium chinense* seeds and *Taxus chinensis* roots were respectively collected, followed by air dried under sunlight for 72 h. And then, all samples were immediately frozen by liquid nitrogen and kept at -80°C until analysis.

Metabolites extraction

All samples were grounded in liquid nitrogen into fine powders by SPEX 6870 Freezer/Mill (SPEX SamplePrep, New Jersey, USA) and about 50 mg of samples was transferred into 2 mL centrifuge tubes. 0.4 mL extraction liquid ($V_{methanol}$:V_{H2O} = 3:1) and 20 μL of Adonitol (1 mg/mL stock in dH_2O, internal standard) were then added and mixed for about 30 s. After homogenizing for 5 min, the mixture was centrifuged at 13,000 × g for 15 min in 4°C. And then 0.4 mL of the supernatant was transferred into a fresh 2 mL GC/MS glass vial. After drying in a vacuum concentrator without heating, the extracts were incubated in 80 μL methoxyamination hydrochloride (20 mg/mL in pyridine) for 0.5 h at 80°C. Finally, 100 μL BSTFA reagent (1% TMCS, v/v, REGIS Technologies. Inc. USA) was added and incubated at 70°C for 2 h, until further GC-MS analysis.

Metabolites profiling and identification

In the present study, an Agilent 7890 gas chromatograph system (Agilent 7890A, Agilent, USA) combined with a Pegasus 4D time-of-flight mass spectrometer (LECO ChromaTOF PEGASUS 4D, LECO, USA) was employed for metabolic profiling. The system utilized a DB-5MS capillary column coated with 5% diphenyl cross-linked with 95% dimethylpolysiloxane (30 m × 250 μm inner diameter, 0.25 μm film thickness; J & W Scientific, Folsom, CA, USA). A 1 μL aliquot of the analyte was injected in splitless mode. Helium was used as the carrier gas, the

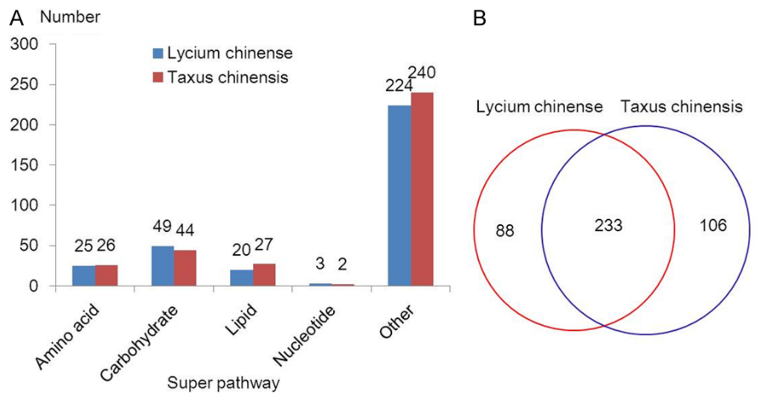

Figure 1. The distribution of metabolites detected in *Lycium chinense* and *Taxus chinensis.*

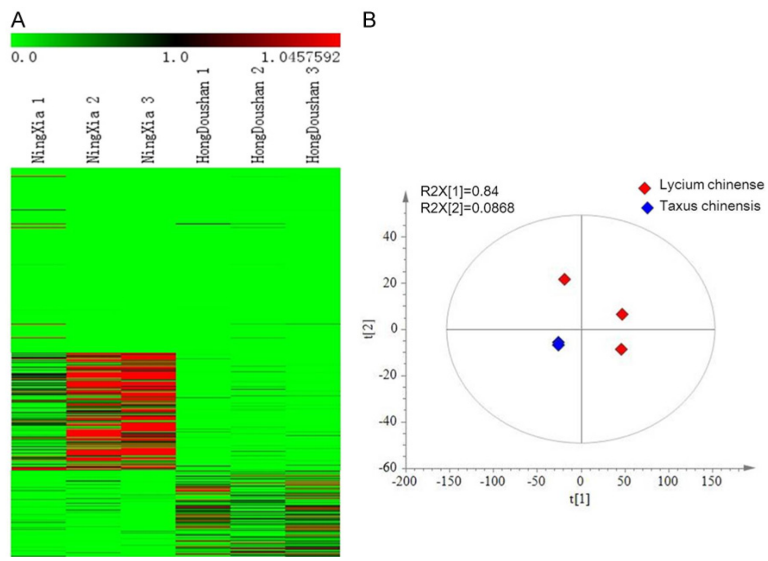

Figure 2. Metabolic variation between *Lycium chinense* and *Taxus chinensis.* A. Heat map representation of 263 metabolites across 6 samples by K-Medians clustering analysis. Each line in the heat map represents a metabolite. The deeper the red color, the higher its content in the tested sample; similarly, the deeper the green color, the lower its content in the tested sample. NingXia 1, NingXia 2, and NingXia 3 were *Lycium chinense*, while HongDoushan 1, HongDoushan 2, and HongDoushan 3 were *Taxus chinensis*. B. PCA scores plot generated from all 427 metabolites cross all 6 samples.

front inlet purge flow was 3 mL/min, and the gas flow rate through the column was 1 mL/min. The initial temperature was kept at 50°C for 1 min, then raised to 300°C at a rate of 10°C/min, then kept for 8min at 300°C. The injection, transfer line, and ion source temperatures were 280, 270 and 220°C, respectively. The energy was -70 eV in electron impact mode. The mass spectrometry data were acquired in full-scan mode with the m/z range of 50-500 at a rate of 20 spectra per second after a solvent delay of 460 s. Meanwhile, Chroma TOF4.3X software of LECO Corporation and LECO-Fiehn Rtx5 database were used for raw peaks exacting and metabolites identification as our previous reports [11].

Metabolomic data analysis

Data normalization was performed as described previously [11]. Missing values (if any) were putative to be under the limits of detection and were imputed by the observed minimum. Mev (MultiExperiment Viewer) 4.8 was used for K-Medians clustering analysis while principle component analysis (PCA) analysis was performed with SIMCA-P 13.0 software. Moreover in combination with independent t test (SPSS 17.0 software), partial least squares discriminant analysis (PLS-DA, SIMCA-P 13.0 software) was employed for identifying significant different metabolites [11]. Here metabolites with both VIP values (in PLS-DA model) more than 1 and *p* values (in t tests) less than 0.05 were determined to be significant. The content of each metablites was relative quantification, so in the PLS-DA model, those items uniquely detected in anyone of the two herbs were removed for their highly suspect roles on the separation of the two TCMs.

Results

Metabolic profiling of Lycium chinense

To comprehensively understand the metabolome for *Lycium chinense*, here we employed a non-targeted metabolomics technology GC/TOF MS for metabolic profiling. Totally 321 metabolites were identified in the tested three samples (**Figure 1** and Supplementary Table 1), which included 25 amino acids, 49 carbohydrates, 20 lipids, 3 nucleotides and other 224

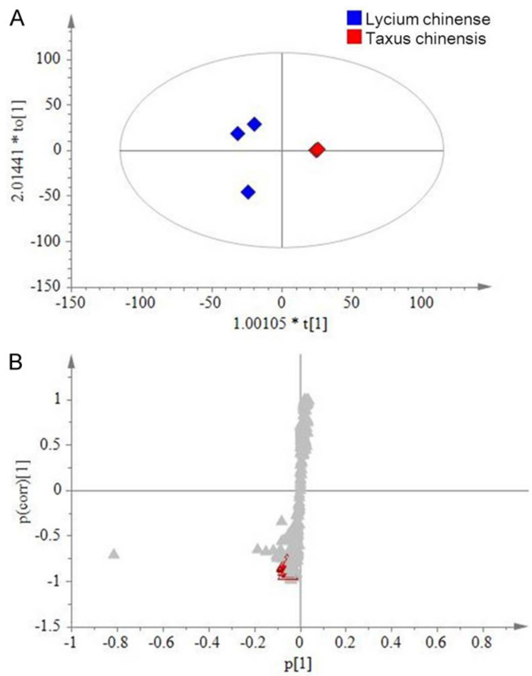

Figure 3. A. Score plot from PLS-DA model of samples between *Lycium chinense* and *Taxus chinensis*. B. S plot from PLS-DA model of samples between *Lycium chinense* and *Taxus chinensis*. Metabolites playing key roles for separation are marked with red triangle.

metabolites. Moreover, 36 named metabolites and 129 metabolites identified as analytes were included in these 224 metabolites, as well as 59 metabolites determined to be unknown. Among these 321 metabolites, those 133 named metabolites covered most of the central metabolism pathways including amino acid, carbohydrate, lipid, and nucleotide super pathway. Especially when compared with previous studies, the result here uncovered so far the broadest metabolome for *Lycium chinense*. Furthermore, the rest unnamed 188 metabolites were supposed to be identified in the future study.

Metabolic profiling of Taxus chinensis

Likewise, by subjecting three samples of *Taxus chinensis* into the abovementioned metabolomic platform, a total of 339 metabolites were identified including 26 amino acids, 44 carbohydrates, 27 lipids, 2 nucleotides and other 240 metabolites (**Figure 1** and Supplementary Table 1). Furthermore, the 240 metabolites included 50 named metabolites and 121 metabolites identified as analytes, while the rest 69 metabolites were determined to be unknown. Totally 427 metabolites were found in *Lycium chinense* and *Taxus chinensis*, while there were more than 18 metabolites detected in *Taxus chinensis* (**Figure 1** and Supplementary Table 1). Moreover, 116 metabolites were only found in *Taxus chinensis*, while 88 metabolites were merely determined in *Lycium chinense*. More importantly, when compared to the other studies, the present study also uncovered so far the broadest metabolome for *Taxus chinensis* and in particular the major metabolism pathways such as amino acid, carbohydrate, lipid, and nucleotide super pathway were covered by 149 named metabolites.

Metabolic variation between Lycium chinense and Taxus chinensis

To determine the metabolic similarities and differences between *Lycium chinense* and *Taxus chinensis*, K-Medians clustering analysis was performed and resulted in a plot of all the 427 biochemicals *vs* 6 samples. As shown in **Figure 2A**, the three *Lycium chinense* samples clustered together, as did the three *Taxus chinensis* samples. Notably, the metabolites at the upper part in the heat-map displayed to be abundance in *Lycium chinense,* while the metabolites at the lower part in the heat-map showed to be enriched in *Taxus chinensis*. Meanwhile, the widely used un-supervised method PCA was then performed to provide a snapshot of the information hidden in the metabolomic data of the tested six samples. Obviously, the three *Lycium chinense* samples could be completely separated from the three *Taxus chinensis* samples **Figure 2B**. The results here showed remarkable diversity in their abundances of biochemicals across the 6 tested samples.

Significantly changed metabolites between Lycium chinense and Taxus chinensis

To further evaluate the metabolic differences between *Lycium chinense* and *Taxus chinensis*, the supervised statistical method PLS-DA was then employed. It was considered to be one of the most effective strategies for metabolomics data analysis, which was suitable for metabolic data that contained more metabolites (in hundreds) than biological samples (only tens) [14]. Likewise, in the model of PLS-DA, three samples from *Lycium chinense* could be completely separated from those from *Taxus chinensis*

Table 1. List of different metabolites between *Lycium chinense* and *Taxus chinensis*, responsible for the separation

Super Pathway	Biochemical Name	R.T. (minutes)	Fold Change	*p* value
Amino acid	Threo-beta-hyrdoxyaspartate 2	16.4064	0.0283	4.78E-02
Carbohydrate	Galactose 2	20.0426	0.0184	3.02E-02
	Gentiobiose 1	27.5839	0.0841	5.14E-02
	Glucose-1-phosphate	18.4482	0.0170	3.75E-02
Others	Arbutin	25.6829	0.0135	4.60E-02
	Unknown 024	18.5344	0.0219	2.69E-02

(**Figure 3A**). Together with independent t tests, further statistical analysis showed that only six metabolites (**Figure 3B** and **Table 1**) were significantly changed (VIP ≥ 1 and $p \leq 0.05$), playing an important role in the separation. Interestingly, all six metabolites displayed high levels in *Lycium chinense* than those in *Taxus chinensis,* whose ratios ranged from 0.0135 to 0.0841. Among them, the level of DL-threo-β-hydroxyaspartate, a known inhibitor of glutamate uptake, was higher in *Lycium chinense* than in *Taxus chinensis* [15]. Galactose was also included, which may be toxic to ovarian germ cells and more importantly, galactose metabolism may be a risk factor for ovarian cancer [16].

Discussion

TCMs have been used in the Chinese health care system for over 2,000 years. And more importantly, a large number of active pharmacological compounds have been isolated from TCMs and identified for whole-body homeostasis and disease prevention [17, 18]. As reported, these bioactive compounds could enhance human health by stimulating blood circulation and/or by supplementing vital energy and treat various diseases including Alzheimer's disease, diabetes, allergy, inflammation, microbial infections, and cancer [19]. For example, *Ginseng*-specific saponins are major bioactive compounds for the metabolic activities [12]. Moreover, berberine, extracted from *rhizoma coptidis*, is reported to be an oral hypoglycemic agent and also functions as anti-obesity and anti-dyslipidemia bioactive compounds [20]. Additionally, bitter melon (*Momordica charantia*) plays key roles in protecting β cells, enhancing insulin sensitivity, reducing blood glucose, lipids and oxidative stress as well [21]. In the present study, metabolic characterizations of two TCMs including *Lycium chinense* and *Taxus chinensis* were investigated by a non-targeted metabolomic technology, GC/TOF MS, which not only uncovered bioactive compounds in these two TCMs, but also provided new insights into their metabolic activities on diseases prevention and treatment.

Lycium chinense (Goji berry or wolfberry) has been commonly used in China as a herbal medicine and tonic for thousands of years [22]. Due to numerous biological activities including immune-regulatory, antioxidant properties, anti-fatigue and antitumor, the consumption of *Lycium chinense* has been demonstrated to have potential pharmaceutical interests particularly associated with eyes, liver, and the kidney [22, 23]. As reported, *Lycium chinense* consists of many compounds (metabolites) including amino acids, essential oils, vitamins, and trace minerals. And especially, two major bio-active components including polysaccharides and carotenoids have been focused, which play key roles on exerting ocular neuroprotective effects, hepatic protection, immunomodulatory and antioxidative effects, and potential antitumor properties [24, 25]. To the best of our knowledge, there are very few studies on its biological activities or bio-active components by metabolomics. We here employed a non-targeted metabolomic technology, GC/TOF MS in order to comprehensively uncover metabolic characterization of *Lycium chinense*. A total of 321 metabolites were identified in *Lycium chinense*, which uncovered so far the broadest metabolome for *Lycium chinense* when compared with previous studies [22, 24, 25]. Among these 321 metabolites, 25 amino acids, 49 carbohydrates, 20 lipids, 3 nucleotides and other 224 metabolites were included. These metabolites in *Lycium chinense* may contribute to its pharmaceutical interests. For example, The *Lycium Barbarum* polysaccharides (LBP) including glucose, galactose and xylose were detected as previous reports [22, 24]. Metabolites such as quinic acid with neuroprotective and neurotrophic effects and arbutin with antioxidative activity were also found in *Lycium chinense* [26, 27]. Moreover, there have been a number of metabolites determined in *Lycium chinense,* which has real potential inhibitory effect on the growth of cancer cells, antibacterial, or functions on lowering blood glucose/cholesterol including canavanine, tartaric acid, myo-inositol, sophorose, xylitol, oleic acid, and linoleic acid [28-32]. Especially, two metabolites including salicin and xanthotoxin, were only detected in *Lycium chinense,* which has anti-inflammatory and analgesic actions or have anti-tumor effects and an anti-inflammatory effect [33, 34].

Taxus chinensis has also been widely recognized as an important TCM since it is reported to have significant inhibitive effects on various cancers including ovarian cancer and central nervous system tumors. In the present study, 339 metabolites in total were identified in the root of *Taxus chinensis* by GC/TOF MS, which uncovered so far the broadest metabolome for *Taxus chinensis* when compared with other studies [35-37]. As well-known, *Taxus chinensis* is a rich source of biological active components including toxoids and diterpenoids, showing significant pharmaceutical interests such as anticancer property, antioxidant activity, anti-adipogenic activity and cardio-protective effect. Among those 339 detected metabolites, quite a few metabolites may play importantly roles on significant pharmaceutical interests, among which certain metabolites were only detected in *Taxus chinensis* rather than *Lycium chinense*. For example, several metabolites such as naringenin, 2-Hydroxyestrone, and phytosphingosine are associated with tumor prevention or could induce apoptotic cell death [38-40]. Moreover, other metabolites including gentisic acid and synephrine have antioxidant activities, while linoleic acid methyl ester is reported to be associated with the generation of reactive oxygen species (ROS) [41].

After comprehensively revealing metabolic characterizations of *Lycium chinense* and *Taxus chinensis*, further analysis indicated remarkable metabolic variation between these two TCMs. More importantly, six significantly changed metabolites (VIP ≥ 1 and $p \leq 0.05$) were determined between *Lycium chinense* and *Taxus chinensis*, which were supposed to discriminate them. Furthermore, these six metabolites may play important roles on their specific significant pharmaceutical interests including anticancer property.

In summary, taking advantage of an un-targeted technology GC-TOF-MS, we comprehensively revealed metabolic characterization of TCMs, *Lycium chinense* and *Taxus chinensis*. More importantly, a series of bio-active components (metabolites) were identified, which may play important roles on their significant pharmaceutical interests including anticancer properties and antioxidant activities. Furthermore, significant metabolic variation and differences were also determined between these two TCMs. The results here may not only extend our understanding on the metabolic characterization of *Lycium chinense* and *Taxus chinensis*, but also provide new data to suppose their significant potentials in diseases treatment and prevention.

Acknowledgements

This work was supported by the funds from the Health and Family Planning Commission of Jiangxi Province (Grant No. 2015A067 and 20171118).

Disclosure of conflict of interest

None.

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Supplementary Table 1. List of 427 detected metabolites with some important properties including CAS, KEGG and PubChem entry numbers

Biochemical Name	Super Pathway	R.T. (minutes)	Detected*	CAS	KEGG	PubChem	Clustering analysis#
Asparagine 3	Amino Acid	16.791	Both	70-47-3	C00152	6267	Class 2
Aspartic acid 2	Amino Acid	14.433	Both	56-84-8	C00049	5960	Class 2
Canavanine degr prod	Amino Acid	11.580	Both				Class 2
L-Allothreonine 1	Amino Acid	13.864	Both	28954-12-3	C05519	7864	Class 2
Leucine	Amino Acid	12.328	Both	61-90-5	C00123	6106	Class 2
3-Aminoisobutyric acid 1	Amino acid	14.893	Both	144-90-1	C05145	64956	Class 2
3-Hydroxynorvaline 2	Amino acid	13.484	Both	2280-42-4			Class 2
4-hydroxybutyrate	Amino acid	11.819	Both	591-81-1			Class 2
Alanine 1	Amino acid	9.879	Both	56-41-7	C01401	602	Class 2
Beta-Alanine 2	Amino acid	14.475	Both	107-95-9	C00099	239	Class 2
Glycine 2	Amino acid	12.850	Both	56-40-6	C00037	750	Class 2
Isoleucine	Amino acid	12.645	Both	73-32-5	C00407	6306	Class 2
N-Ethylglycine 1	Amino acid	14.209	Both	627-01-0	C11735	316542	Class 2
N-Methyl-L-glutamic acid 2	Amino acid	16.239	Both		C01046	4288	Class 2
Oxoproline	Amino acid	15.702	Both	98-79-3	C02238	7405	Class 2
Proline	Amino acid	12.753	Both	147-85-3	C00148	614	Class 2
Serine 1	Amino acid	13.516	Both	56-45-1	C00716	617	Class 2
Threo-beta-hyrdoxyaspartate 2	Amino acid	16.406	Both	4294-45-5			Class 2
Valine	Amino acid	11.540	Both	72-18-4	C00183	1182	Class 2
Cellobiose 2	Carbohydrate	26.881	Both	16462-44-5	C00185	3485	Class 2
Citric acid	Carbohydrate	19.015	Both	5949-29-1	C00158	311	Class 2
D-Glyceric acid	Carbohydrate	13.095	Both	6000-40-4	C00258	752	Class 2
Fructose 1	Carbohydrate	19.525	Both	57-48-7	C10906	5984	Class 2
Fumaric acid	Carbohydrate	13.414	Both	100-17-8	C00122	444972	Class 2
Galactonic acid	Carbohydrate	20.805	Both	576-36-3	C00880	4136	Class 2
Galactose 2	Carbohydrate	20.043	Both	59-23-4	C00124	3424	Class 2
Gentiobiose 1	Carbohydrate	27.584	Both	554-91-6	C08240	10439	Class 2
Glucosaminic acid	Carbohydrate	21.237	Both	3646-68-2	C03752	6511	Class 2
Glucose-1-phosphate	Carbohydrate	18.448	Both	59-56-3	C11450	65533	Class 2
Glucuronic acid 2	Carbohydrate	20.208	Both	1700908	C00191	94715	Class 2
Lactic acid	Carbohydrate	9.222	Both	50-21-5	C01432	612	Class 2
Lactulose 1	Carbohydrate	26.659	Both	4618-18-2	C07064	9276	Class 2
Leucrose 1	Carbohydrate	27.348	Both	71205-61-3			Class 2
L-Malic acid	Carbohydrate	15.179	Both	97-67-6	C00149	222656	Class 2
L-Threose 1	Carbohydrate	14.711	Both	95-44-3		101562	Class 2
Lyxose 1	Carbohydrate	17.152	Both	1114-34-7	C00476	3759	Class 2
Maltose	Carbohydrate	27.195	Both	69-79-4	C00208	3508	Class 2
Myo-inositol	Carbohydrate	21.746	Both	87-89-8	C06153	892	Class 2
N-Acetyl-beta-D-mannosamine 4	Carbohydrate	21.880	Both	3615-17-6	C00645	3918	Class 2
N-Acetyl-D-galactosamine 3	Carbohydrate	21.599	Both	14215-68-0	C01132	35717	Class 2
Oxalic acid	Carbohydrate	10.298	Both	144-62-7	C00209	971	Class 2
Ribose	Carbohydrate	17.456	Both	24259-59-4	C00121	993	Class 2
Sophorose 1	Carbohydrate	27.229	Both	20880-64-2	C08250	10449	Class 2
Succinic acid	Carbohydrate	12.926	Both	110-15-6	C00042	1110	Class 2
Sucrose 1	Carbohydrate	26.217	Both	57-50-1	C00089	5988	Class 3
Sucrose 2	Carbohydrate	26.217	Both	57-50-1	C00089	5988	Class 3
Xylitol	Carbohydrate	17.539	Both	87-99-0	C00379	3669	Class 2
Oleic acid	Lipids	22.897	Both	112-80-1	C00712	3978	Class 2
Oxamic acid	Lipids	12.209	Both	471-47-6	C01444	4622	Class 2
Xanthosine	Nucleotide	26.482	Both	146-80-5	C01762	64959	Class 3
3-hydroxybutyric acid	Others	10.714	Both	306-31-0		441	Class 2
Analyte 112	Others	14.263	Both				Class 2
Analyte 129	Others	15.404	Both				Class 3
Analyte 13	Others	8.057	Both				Class 2
Analyte 14	Others	8.068	Both				Class 2
Analyte 140	Others	16.356	Both				Class 2
Analyte 147	Others	16.653	Both				Class 3
Analyte 158	Others	17.406	Both				Class 2
Analyte 17	Others	8.161	Both				Class 3

Analyte 233	Others	20.904	Both				Class 3
Analyte 236	Others	21.021	Both				Class 2
Analyte 27	Others	8.627	Both				Class 3
Analyte 29	Others	8.749	Both				Class 3
Analyte 3	Others	7.788	Both				Class 3
Analyte 303	Others	23.894	Both				Class 3
Analyte 324	Others	24.865	Both				Class 2
Analyte 330	Others	25.107	Both				Class 2
Analyte 42	Others	9.321	Both				Class 3
Analyte 49	Others	9.649	Both				Class 2
Analyte 5	Others	7.838	Both				Class 2
Analyte 50	Others	9.672	Both				Class 2
Analyte 51	Others	9.759	Both				Class 2
Analyte 69	Others	10.932	Both				Class 3
Analyte 74	Others	11.224	Both				Class 1
Analyte 75	Others	11.248	Both				Class 2
Analyte 93	Others	12.650	Both				Class 1
Benzoic acid	Others	12.126	Both	65-85-0	C03096	243	Class 3
Phosphate 1	Others	12.321	Both	7664-38-2	C00009	1004	Class 2
Tartaric acid	Others	16.953	Both	133-37-9	C00898	875	Class 3
Toluenesulfonic acid	Others	16.963	Both	6192-52-5			Class 1
Unknown 011	Others	12.178	Both				Class 2
Unknown 017	Others	14.538	Both				Class 2
Unknown 018	Others	14.780	Both				Class 2
Unknown 023	Others	18.355	Both				Class 2
Unknown 025	Others	18.732	Both				Class 2
Unknown 051	Others	22.840	Both				Class 2
Unknown 069	Others	26.775	Both				Class 1
Unknown 074	Others	27.329	Both				Class 3
Unknown 078	Others	27.995	Both				Class 3
Unknown 084	Others	28.646	Both				Class 3
Unknown 086	Others	28.786	Both				Class 2
4-aminobutyric acid 1	Amino acid	15.776	Both	20791	C00334	3628	Class 3
3-Hydroxypropionic acid 1	Carbohydrate	10.438	Both	503-66-2	C01013	68152	Class 3
Beta-Mannosylglycerate 2	Carbohydrate	19.280	Both	164324-35-0		5460194	Class 3
D-Arabitol	Carbohydrate	17.936	Both	488-82-4		94154	Class 3
Fructose 2,6-biphosphate degr prod 2	Carbohydrate	22.776	Both				Class 3
Isomaltose 2	Carbohydrate	28.038	Both	499-40-1	C00252	3551	Class 3
Pyruvic acid	Carbohydrate	9.077	Both	127-17-3	C00022	1060	Class 3
Sorbitol	Carbohydrate	20.239	Both	50-70-4	D00096	5780	Class 3
Xylose 2	Carbohydrate	17.205	Both	6763-34-4		644160	Class 2
Ethanolamine	Lipids	12.290	Both	141-43-5	C00189	700	Class 3
Prunin degr. Prod. 1	Lipids	27.839	Both	529-55-5	C09099	11291	Class 2
Resveratrol 1	Lipids	26.940	Both	501-36-0	C03582	6374	Class 3
3-Hydroxypyridine	Others	10.542	Both	109-00-2		7971	Class 2
Analyte 12	Others	8.061	Both				Class 2
Analyte 149	Others	16.762	Both				Class 2
Analyte 16	Others	8.155	Both				Class 2
Analyte 18	Others	8.196	Both				Class 2
Analyte 19	Others	8.227	Both				Class 2
Analyte 2	Others	7.773	Both				Class 3
Analyte 21	Others	8.418	Both				Class 3
Analyte 22	Others	8.518	Both				Class 3
Analyte 255	Others	22.049	Both				Class 3
Analyte 270	Others	22.552	Both				Class 2
Analyte 271	Others	22.654	Both				Class 3
Analyte 28	Others	8.720	Both				Class 3
Analyte 283	Others	23.120	Both				Class 3
Analyte 313	Others	24.314	Both				Class 3
Analyte 358	Others	26.318	Both				Class 2
Analyte 407	Others	29.106	Both				Class 2
Analyte 417	Others	30.414	Both				Class 2
Analyte 428	Others	32.411	Both				Class 3

Analyte 54	Others	9.977	Both				Class 2
Analyte 55	Others	10.105	Both				Class 3
Analyte 61	Others	10.475	Both				Class 3
Analyte 66	Others	10.758	Both				Class 3
Analyte 77	Others	11.422	Both				Class 2
Analyte 8	Others	7.882	Both				Class 3
Arbutin	Others	25.683	Both	497-76-7	C06186	8437	Class 2
Glycolic acid	Others	9.465	Both	79-14-1	C03547	757	Class 2
Hydroxylamine	Others	10.119	Both	7803-49-8	C00192	787	Class 3
Iminodiacetic acid	Others	15.727	Both	142-73-4			Class 3
Sulfuric acid	Others	10.801	Both	7664-93-9	C00059	1118	Class 3
Unknown 001	Others	9.035	Both				Class 2
Unknown 004	Others	9.31	Both				Class 3
Unknown 006	Others	9.931	Both				Class 3
Unknown 027	Others	18.986	Both				Class 2
Unknown 062	Others	25.705	Both				Class 3
Unknown 072	Others	27.044	Both				Class 3
Unknown 076	Others	27.447	Both				Class 2
Glucose 1	Carbohydrate	19.820	Both	50-99-7	C00031	79025	Class 1
Tagatose 2	Carbohydrate	19.520	Both	87-81-0		92092	Class 2
1-Monopalmitin	Lipids	25.847	Both	19670-51-0			Class 3
Abietic Acid 2	Lipids	24.360	Both	514-10-3	C06087	8353	Class 3
Galactinol 2	Lipids	28.032	Both	3687-64-7	C01235	4456	Class 3
Linoleic acid	Lipids	22.850	Both	112-63-0		5284421	Class 2
Malonic acid 1	Lipids	11.356	Both	141-82-2	C04025	867	Class 2
Palmitic acid	Lipids	21.331	Both	21096	C00249	985	Class 2
Piceatannol 2	Lipids	25.491	Both	10083-24-6	C05901	8189	Class 3
Stearic acid	Lipids	23.112	Both	21128	C01530	5281	Class 3
(2R, 3S)-2-hydroxy-3-isopropylbutanedioic acid	Others	16.241	Both	3237-44-3		5516	Class 2
2-amino-2-methylpropane-1,3-diol 2	Others	10.949	Both	115-69-5			Class 1
2-hydroxypyridine	Others	8.96	Both	142-08-5	C02502	8871	Class 2
5-Dihydrocortisol 2	Others	30.174	Both	1482-50-4			Class 3
Analyte 1	Others	7.705	Both				Class 3
Analyte 11	Others	8.006	Both				Class 3
Analyte 124	Others	14.979	Both				Class 3
Analyte 134	Others	15.702	Both				Class 2
Analyte 143	Others	16.462	Both				Class 2
Analyte 15	Others	8.107	Both				Class 3
Analyte 181	Others	19.072	Both				Class 3
Analyte 20	Others	8.419	Both				Class 3
Analyte 222	Others	20.511	Both				Class 3
Analyte 237	Others	21.083	Both				Class 2
Analyte 24	Others	8.555	Both				Class 3
Analyte 246	Others	21.526	Both				Class 3
Analyte 25	Others	8.587	Both				Class 2
Analyte 26	Others	8.625	Both				Class 3
Analyte 268	Others	22.468	Both				Class 2
Analyte 273	Others	22.756	Both				Class 3
Analyte 280	Others	23.044	Both				Class 3
Analyte 286	Others	23.282	Both				Class 3
Analyte 294	Others	23.592	Both				Class 2
Analyte 30	Others	8.812	Both				Class 2
Analyte 305	Others	23.951	Both				Class 2
Analyte 31	Others	8.848	Both				Class 3
Analyte 315	Others	24.424	Both				Class 3
Analyte 32	Others	8.912	Both				Class 3
Analyte 326	Others	24.968	Both				Class 2
Analyte 333	Others	25.231	Both				Class 2
Analyte 340	Others	25.408	Both				Class 2
Analyte 342	Others	25.413	Both				Class 3
Analyte 350	Others	25.979	Both				Class 3
Analyte 36	Others	9.117	Both				Class 3
Analyte 38	Others	9.212	Both				Class 3

Analyte 4	Others	7.820	Both				Class 3
Analyte 408	Others	29.199	Both				Class 3
Analyte 418	Others	30.645	Both				Class 3
Analyte 420	Others	30.764	Both				Class 2
Analyte 43	Others	9.375	Both				Class 3
Analyte 45	Others	9.436	Both				Class 3
Analyte 59	Others	10.342	Both				Class 3
Analyte 7	Others	7.845	Both				Class 2
Analyte 73	Others	11.175	Both				Class 3
Analyte 80	Others	11.607	Both				Class 3
Analyte 9	Others	7.901	Both				Class 3
Cis-gondoic acid	Others	24.582	Both	5561-99-9		5282768	Class 2
Dehydroascorbic Acid 2	Others	19.599	Both	490-83-5	C01041	4283	Class 2
Digitoxose 1	others	16.538	Both	527-52-6	C21045	254816270	Class 2
DL-dihydrosphingosine 1	Others	25.029	Both	13552-09-5		3126	Class 2
Gluconic acid 1	Others	20.844	Both	527-07-1	C00257	10690	Class 2
Hesperitin 1	Others	28.719	Both	520-33-2			Class 3
IS	Others	17.987	Both				Class 3
Methyl Phosphate	Others	10.988	Both	7023-27-0		13130	Class 3
Phosphate 2	Others	12.310	Both	7664-38-2	C00009	1004	Class 2
Quinic acid	Others	19.405	Both	77-95-2	C00296	6508	Class 2
Resorcinol	Others	13.895	Both	108-46-3	C01751	5054	Class 2
Tartronic acid	Others	13.838	Both	80-69-3	C02500	45	Class 2
Threonic acid	Others	16.027	Both	7306-96-9		151152	Class 2
Unknown 003	Others	9.268	Both				Class 3
Unknown 007	Others	10.111	Both				Class 3
Unknown 008	Others	10.543	Both				Class 3
Unknown 012	Others	12.762	Both				Class 2
Unknown 013	Others	13.056	Both				Class 2
Unknown 019	Others	15.589	Both				Class 2
Unknown 020	Others	17.704	Both				Class 2
Unknown 024	Others	18.534	Both				Class 2
Unknown 029	Others	19.243	Both				Class 3
Unknown 033	Others	19.948	Both				Class 2
Unknown 038	Others	20.419	Both				Class 1
Unknown 039	Others	20.715	Both				Class 3
Unknown 045	Others	22.082	Both				Class 2
Unknown 046	Others	22.141	Both				Class 2
Unknown 053	Others	23.314	Both				Class 2
Unknown 058	Others	24.827	Both				Class 1
Unknown 063	Others	26.179	Both				Class 3
unknown 064	Others	26.192	Both				Class 3
Unknown 068	Others	26.741	Both				Class 2
Unknown 071	Others	26.942	Both				Class 2
Unknown 080	Others	28.266	Both				Class 2
Unknown 081	Others	28.334	Both				Class 2
Unknown 087	Others	29.259	Both				Class 3
Uun	Others	15.990	Both				Class 2
Threitol	Carbohydrate	15.256	Lycium chinense	7493-90-5		169019	Class 1
Neohesperidin	Lipids	25.122	Lycium chinense	13241-33-3	C09806	11994	Class 1
Prostaglandin A2 1	Lipids	26.271	Lycium chinense	8237	C05953	27820	Class 1
Analyte 111	Others	14.089	Lycium chinense				Class 1
Analyte 135	Others	15.840	Lycium chinense				Class 1
Analyte 267	Others	22.498	Lycium chinense				Class 1
Analyte 339	Others	25.399	Lycium chinense				Class 1
Analyte 413	Others	29.452	Lycium chinense				Class 1
Analyte 48	Others	9.543	Lycium chinense				Class 1
D-erythronolactone 1	Others	14.533	Lycium chinense	15667-21-7			Class 1
Unknown 010	Others	11.715	Lycium chinense				Class 1
Unknown 015	Others	13.599	Lycium chinense				Class 1
Unknown 016	Others	14.247	Lycium chinense				Class 1
Unknown 044	Others	22.104	Lycium chinense				Class 1
Unknown 049	Others	22.370	Lycium chinense				Class 1

Uridine 1	Nucleotide	24.988	Lycium chinense	58-96-8	C00299	6029	Class 1
Analyte 107	Others	13.851	Lycium chinense				Class 1
Analyte 125	Others	15.047	Lycium chinense				Class 1
Analyte 238	Others	21.110	Lycium chinense				Class 1
Analyte 269	Others	22.556	Lycium chinense				Class 1
Analyte 279	Others	23.013	Lycium chinense				Class 1
Analyte 281	Others	23.078	Lycium chinense				Class 1
Analyte 289	Others	23.436	Lycium chinense				Class 1
Analyte 299	Others	23.743	Lycium chinense				Class 1
Analyte 302	Others	23.862	Lycium chinense				Class 1
Analyte 309	Others	24.122	Lycium chinense				Class 1
Analyte 312	Others	24.307	Lycium chinense				Class 1
Analyte 319	Others	24.644	Lycium chinense				Class 1
Analyte 341	Others	25.443	Lycium chinense				Class 1
Analyte 348	Others	25.931	Lycium chinense				Class 1
Analyte 397	Others	28.601	Lycium chinense				Class 1
Analyte 419	Others	30.766	Lycium chinense				Class 1
Analyte 427	Others	32.030	Lycium chinense				Class 1
Analyte 72	Others	11.070	Lycium chinense				Class 1
Hydantoin, 5-(4-hydroxybutyl)- 2	Others	20.302	Lycium chinense	461-72-3			Class 1
Salicin	Others	25.321	Lycium chinense	138-52-3		5145	Class 1
Unknown 060	Others	25.327	Lycium chinense				Class 1
Unknown 061	Others	25.756	Lycium chinense				Class 1
Canavanine 1	Amino Acid	20.591	Lycium chinense	543-38-4	C00308	3602	Class 1
Homocystine 2	Amino Acid	25.258	Lycium chinense	626-72-2	C01817	4941	Class 1
N-Acetyl-L-aspartic acid 2	Amino Acid	17.229	Lycium chinense	997-55-7; 997-55-7	C01042	65065	Class 1
2,4-diaminobutyric acid 3	Amino acid	14.651	Lycium chinense	1758-80-1	C03283	6142	Class 1
N-Methyl-DL-alanine	Amino acid	10.906	Lycium chinense	600-21-5		4377	Class 1
1-Kestose	Carbohydrate	31.563	Lycium chinense	470-69-9	G00339		
2-Deoxy-D-galactose 2	Carbohydrate	18.825	Lycium chinense	1949-89-9		225612	Class 1
2-Keto-L-gulonic acid	Carbohydrate	19.886	Lycium chinense	526-98-7	C15673	47204999	Class 1
3,6-Anhydro-D-galactose 3	Carbohydrate	18.298	Lycium chinense	14122-18-0	C06474	441040	Class 1
D-galacturonic acid 2	Carbohydrate	20.530	Lycium chinense	685-73-4	C00333	3627	Class 1
d-Glucoheptose 2	Carbohydrate	22.268	Lycium chinense	62475-58-5		219662	Class 1
Erythrose 2	Carbohydrate	14.457	Lycium chinense	583-50-6		94176	Class 1
Fructose-6-phosphate	Carbohydrate	23.554	Lycium chinense	643-13-0		69507	Class 1
Glucoheptonic acid 1	Carbohydrate	23.158	Lycium chinense	23351-51-1			Class 1
Lactose 2	Carbohydrate	26.509	Lycium chinense	63-42-3		493593	Class 1
2-Deoxyerythritol	Lipids	12.619	Lycium chinense	3068-00-6			Class 1
Behenic acid	Lipids	26.419	Lycium chinense	112-85-6	C08281	10479	Class 1
Beta-Hydroxymyristic acid	Lipids	21.209	Lycium chinense	1961-72-4			Class 1
Naringin	Lipids	31.222	Lycium chinense	10236-47-2	C09789	11977	Class 1
Pipecolinic acid	Lipids	13.686	Lycium chinense	3105-95-1	C00408	3698	Class 1
Purine riboside	Nucleotide	24.079	Lycium chinense	550-33-4	C01736	68368	Class 1
1,4-Cyclohexanedione 1	Others	12.895	Lycium chinense	637-88-7	C08063	12511	Class 1
Analyte 10	Others	7.931	Lycium chinense				Class 1
Analyte 228	Others	20.779	Lycium chinense				Class 1
Analyte 298	Others	23.695	Lycium chinense				Class 1
Analyte 300	Others	23.803	Lycium chinense				Class 1
Analyte 301	Others	23.828	Lycium chinense				Class 1
Analyte 306	Others	24.023	Lycium chinense				Class 1
Analyte 316	Others	24.509	Lycium chinense				Class 1
Analyte 317	Others	24.559	Lycium chinense				Class 1
Analyte 320	Others	24.649	Lycium chinense				Class 1
Analyte 338	Others	25.338	Lycium chinense				Class 1
Analyte 351	Others	26.004	Lycium chinense				Class 1
Analyte 396	Others	28.540	Lycium chinense				Class 1
Analyte 410	Others	29.281	Lycium chinense				Class 1
Analyte 412	Others	29.391	Lycium chinense				Class 1
Noradrenaline	Others	22.407	Lycium chinense	51-41-2	C00547	3828	Class 1
Trans-3,5-Dimethoxy-4-hydroxycinnamaldehyde 1	Others	22.039	Lycium chinense	4206-58-0			Class 1
Unknown 014	Others	13.363	Lycium chinense				Class 1
Unknown 036	Others	20.352	Lycium chinense				Class 1

Unknown 041	Others	21.311	Lycium chinense				Class 1
Unknown 048	Others	22.345	Lycium chinense				Class 1
Unknown 050	Others	22.700	Lycium chinense				Class 1
Unknown 052	Others	23.189	Lycium chinense				Class 1
Unknown 054	Others	23.533	Lycium chinense				Class 1
Unknown 056	Others	23.659	Lycium chinense				Class 1
Unknown 057	Others	24.243	Lycium chinense				Class 1
Unknown 059	Others	25.191	Lycium chinense				Class 1
Unknown 065	Others	26.549	Lycium chinense				Class 1
Xanthotoxin 2	Others	23.518	Lycium chinense	298-81-7	C01864	4978	Class 1
Heptadecanoic acid	Lipids	22.232	Taxus chinensis	506-12-7		10465	Class 1
Linoleic acid methyl ester	Lipids	21.810	Taxus chinensis	112-63-0		5284421	Class 1
2-hydroxy-3-isopropylbutanedioic acid	Others	16.350	Taxus chinensis	3237-44-3		5516	Class 1
3,4-dihydroxybenzoic acid	Others	19.082	Taxus chinensis	99-50-3	C00230	3529	Class 1
Analyte 154	Others	17.089	Taxus chinensis				Class 1
Analyte 187	Others	19.243	Taxus chinensis				Class 1
Analyte 248	Others	21.595	Taxus chinensis				Class 1
Analyte 321	Others	24.674	Taxus chinensis				Class 1
Analyte 328	Others	25.006	Taxus chinensis				Class 1
Analyte 357	Others	26.374	Taxus chinensis				Class 1
Analyte 404	Others	28.919	Taxus chinensis				Class 1
Cortexolone 4	Others	30.211	Taxus chinensis	152-58-9			Class 1
Dithioerythritol	others	19.478	Taxus chinensis	6892-68-8	C00950	4201	Class 1
Gentisic acid	Others	18.659	Taxus chinensis	490-79-9	C00628	3901	Class 1
Gluconic lactone 1	Others	19.683	Taxus chinensis	90-80-2	C00198	3498	Class 1
Phenyl beta-D-glucopyranoside	Others	23.507	Taxus chinensis	1464-44-4	C11611	13776	Class 1
Phthalic acid	Others	17.653	Taxus chinensis	88-99-3	C01606	4759	Class 1
Synephrine 3	Others	20.849	Taxus chinensis	34520	C04548	7172	Class 1
Unknown 009	Others	10.64	Taxus chinensis				Class 1
Unknown 021	Others	18.105	Taxus chinensis				Class 1
Unknown 022	Others	18.212	Taxus chinensis				Class 1
Unknown 031	Others	19.689	Taxus chinensis				Class 1
Unknown 043	Others	21.797	Taxus chinensis				Class 1
Unknown 066	Others	26.574	Taxus chinensis				Class 1
Unknown 079	Others	28.031	Taxus chinensis				Class 1
4-Androsten-11beta-ol-3,17-dione 1	Lipids	29.031	Taxus chinensis	382-44-5	C05284	7671	Class 1
Epicatechin	Lipids	27.958	Taxus chinensis	490-46-0	C09727	11915	Class 1
Phytosphingosine 1	Lipids	25.933	Taxus chinensis	554-62-1	C12144	14291	Class 1
Alpha-Ecdysone 1	Others	31.434	Taxus chinensis	3604-87-3	C00477	3760	Class 1
Analyte 144	Others	16.527	Taxus chinensis				Class 1
Analyte 203	Others	19.863	Taxus chinensis				Class 1
Analyte 230	Others	20.802	Taxus chinensis				Class 1
Analyte 243	Others	21.316	Taxus chinensis				Class 1
Analyte 253	Others	21.984	Taxus chinensis				Class 1
Analyte 373	Others	27.087	Taxus chinensis				Class 1
Analyte 44	Others	9.49	Taxus chinensis				Class 1
Analyte 6	Others	7.823	Taxus chinensis				Class 1
Analyte 83	Others	12.136	Taxus chinensis				Class 1
L-Gulonolactone	Others	20.036	Taxus chinensis	1128-23-0	C05410	439373	Class 1
Unknown 002	Others	9.116	Taxus chinensis				Class 1
Unknown 005	Others	9.46	Taxus chinensis				Class 1
Unknown 037	Others	20.338	Taxus chinensis				Class 1
Unknown 070	Others	26.851	Taxus chinensis				Class 1
Unknown 082	Others	28.622	Taxus chinensis				Class 1
Unknown 085	Others	28.830	Taxus chinensis				Class 1
Atropine	Amino Acid	23.596	Taxus chinensis	51-55-8	C01479	4651	Class 1
2,6-Diaminopimelic acid 1	Amino acid	20.673	Taxus chinensis	583-93-7	C00680	865	Class 1
N-Acetyltryptophan 4	Amino acid	24.77	Taxus chinensis	87-32-1		2002	Class 1
Putrescine 1	Amino acid	19.879	Taxus chinensis	110-60-1	C00134	1045	Class 1
Trans-4-hydroxy-L-proline 3	Amino acid	15.079	Taxus chinensis	51-35-4	C01157	5810	Class 1
Tyrosine 1	Amino acid	20.229	Taxus chinensis	60-18-4	C01536	1153	Class 1
Galactose 1	Carbohydrate	19.732	Taxus chinensis	59-23-4	C00124	3424	Class 1
Glucose-6-phosphate 2	Carbohydrate	23.938	Taxus chinensis	103192-55-8	C00668	5958	Class 1

Guanidinosuccinic acid 3	Carbohydrate	20.970	Taxus chinensis	6133-30-8		97856	Class 1
Maltotriose 2	Carbohydrate	32.925	Taxus chinensis	1109-28-0	C01835	4954	Class 1
Melibiose 1	Carbohydrate	27.901	Taxus chinensis	585-99-9	C05402	7769	Class 1
Sedoheptulose	Carbohydrate	20.303	Taxus chinensis	3019-74-7	C02076	5162	Class 1
2-Hydroxyestrone	Lipids	28.154	Taxus chinensis	362-06-1	C05298	7682	Class 1
3-hydroxy-3-methylglutaric acid	Lipids	16.585	Taxus chinensis	503-49-1	C03761	6518	Class 1
Allo-inositol	Lipids	19.562	Taxus chinensis	643-10-7			Class 1
Arachidic acid	Lipids	24.754	Taxus chinensis	506-30-9	C06425	8660	Class 1
D-(glycerol 1-phosphate)	Lipids	18.354	Taxus chinensis	34363-28-5	C00093	439162	Class 1
Diglycerol 1	Lipids	18.286	Taxus chinensis	627-82-7		42953	Class 1
Myristic Acid	Lipids	19.392	Taxus chinensis	544-63-8	C06424	11005	Class 1
Naringenin 1	Lipids	28.235	Taxus chinensis	480-41-1	C00509	3792	Class 1
Tetrahydrocorticosterone 3	Lipids	28.978	Taxus chinensis	68-42-8	C05476	7836	Class 1
2'-deoxyadenosine 5'-monophosphate	Nucleotide	29.618	Taxus chinensis	653-63-4	C00360	3651	Class 1
21-hydroxypregnenolone 2	Others	29.374	Taxus chinensis	1164-98-3	C05485	7845	Class 1
2-amino-3-(4-hydroxyphenyl)propanoic acid 1	Others	20.044	Taxus chinensis	6049-54-3			Class 1
2-mercaptoethanesulfonic acid 2	Others	16.706	Taxus chinensis	3375-50-6	C03576	598	Class 1
5-Hydroxyindole-2-carboxylic acid 1	Others	22.826	Taxus chinensis	21598-06-1			Class 1
Analyte 151	Others	16.813	Taxus chinensis				Class 1
Analyte 184	Others	19.168	Taxus chinensis				Class 1
Analyte 185	Others	19.214	Taxus chinensis				Class 1
Analyte 23	Others	8.541	Taxus chinensis				Class 1
Analyte 240	Others	21.237	Taxus chinensis				Class 1
Analyte 287	Others	23.327	Taxus chinensis				Class 1
Analyte 308	Others	24.094	Taxus chinensis				Class 1
Analyte 311	Others	24.268	Taxus chinensis				Class 1
Analyte 336	Others	25.321	Taxus chinensis				Class 1
Analyte 382	Others	27.618	Taxus chinensis				Class 1
Analyte 395	Others	28.516	Taxus chinensis				Class 1
Analyte 421	Others	30.988	Taxus chinensis				Class 1
Analyte 423	Others	31.269	Taxus chinensis				Class 1
Analyte 426	Others	31.766	Taxus chinensis				Class 1
Conduritol b epoxide 2	Others	20.414	Taxus chinensis	6090-95-5		2859	Class 1
Coniferyl alcohol	Others	20.314	Taxus chinensis	32811-40-8; 458-35-5	C00590	3869	Class 1
Dihydrocoumarin 1	others	17.727	Taxus chinensis	119-84-6	C02274	5334	Class 1
Gallic acid	Others	20.390	Taxus chinensis	149-91-7	C01424	4609	Class 1
Octadecanol	Others	22.338	Taxus chinensis	112-92-5			Class 1
Shikimic acid	Others	18.874	Taxus chinensis	138-59-0	C00493	3776	Class 1
Unknown 026	Others	18.627	Taxus chinensis				Class 1
Unknown 028	Others	19.145	Taxus chinensis				Class 1
Unknown 030	Others	19.674	Taxus chinensis				Class 1
Unknown 032	Others	19.696	Taxus chinensis				Class 1
Unknown 034	Others	20.131	Taxus chinensis				Class 1
Unknown 035	Others	20.276	Taxus chinensis				Class 1
Unknown 040	Others	20.953	Taxus chinensis				Class 1
Unknown 042	Others	21.489	Taxus chinensis				Class 1
Unknown 047	Others	22.193	Taxus chinensis				Class 1
Unknown 055	Others	23.631	Taxus chinensis				Class 1
Unknown 067	Others	26.628	Taxus chinensis				Class 1
Unknown 073	Others	27.172	Taxus chinensis				Class 1
Unknown 075	Others	27.447	Taxus chinensis				Class 1
Unknown 077	Others	27.819	Taxus chinensis				Class 1
Unknown 083	Others	28.673	Taxus chinensis				Class 1

*: *Both* means metabolites detected in both *Lycium chinense* and *Taxus chinensis*. *Lycium chinense* means metabolites only detected in Lycium chinense, while *Taxus chinensis* means metabolites detected in *Taxus chinensis*. #: Classification by K-Medians clustering analysis.